

But-2-enamide, N-heptyl-N-octyl-3-methyl-

Inchi:	InChI=1S/C20H39NO/c1-5-7-9-11-13-15-17-21(20(22)18-19(3)4)16-14-12-10-8-6-2/h18H
InchiKey:	HONXCGAHADSTFL-UHFFFAOYSA-N
Formula:	C20H39NO
SMILES:	CCCCCCCCN(CCCCCC)C(=O)C=C(C)C
Mol. weight [g/mol]:	309.53

Physical Properties

Property code	Value	Unit	Source
gf	171.05	kJ/mol	Joback Method
hf	-393.75	kJ/mol	Joback Method
hfus	51.07	kJ/mol	Joback Method
hvap	68.94	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	6.112		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1096.44	kPa	Joback Method
rinpol	2195.00		NIST Webbook
tb	727.35	K	Joback Method
tc	901.72	K	Joback Method
tf	378.52	K	Joback Method
vc	1.161	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.40	J/mol×K	727.35	Joback Method
cpg	915.06	J/mol×K	756.41	Joback Method
cpg	933.77	J/mol×K	785.47	Joback Method
cpg	951.60	J/mol×K	814.53	Joback Method
cpg	968.58	J/mol×K	843.60	Joback Method
cpg	984.76	J/mol×K	872.66	Joback Method
cpg	1000.18	J/mol×K	901.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308241&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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